Comprehensive Descriptors

For Structural and

Statistical Analysis

CODESSA PRO

User's manual

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INTRODUCTION

CODESSA PRO is an entirely new software package, which performs tasks similar to CODESSA, but with many distinct advantages over the previous software package. In particular, its add-in mechanism makes CODESSA PRO expandable, its calculation engine has been optimized at the assembly language level for Pentium, Pentium Pro, Pentium II, Pentium III and Pentium IV processors, and finally, it has been designed to run in 32-bit Windows environments. CODESSA (Comprehensive Descriptors for Structural and Statistical Analysis) PRO is a comprehensive program for developing quantitative structure/property relationships (QSPR), integrating all necessary mathematical and computational tools to (i)calculate a large variety of molecular descriptors on the basis of the 3D geometrical and/or quantum-chemical structural input of chemical compounds; (ii) develop (multi)linear and non-linear QSPR models of the chemical, physical or biological properties of individual compounds (non-linear QSPR models are still in preparation); (iii) perform cluster analyses of the experimental data and molecular descriptors; (iv) interpret the developed models, and (v) predict properties for compounds previously unknown or unavailable.

This manual presents the guidelines for the successful development of a QSAR/QSPR models using the CODESSA PRO program. The execution of each step of the program normally requires knowledge of the proceeding steps, and the steps are therefore discussed in the sequence in which they would be accomplished. This manual also provides further information concerning the features and methods available in the CODESSA PRO program, their purpose, and the interpretation of the results. For a more detailed description of the program and the techniques employed, please refer to the CODESSA PRO *Reference Manual*.

The CODESSA PRO program is designed to operate in the following Microsoft Windows environments: Windows 2000, Windows XP, Windows NT and Windows 9x. To start CODESSA PRO, double click on its icon shown above. When the program starts, the CODESSA PRO Visual Interface (CVI) window will open. Click **Calculate** on the menu-bar to open a pull-down menu, next click on the **Load storage** option to refresh the current snapshot, which is then displayed on the screen. Alternatively, the single keystroke **F5** will refresh the snapshot. Before attempting to use CODESSA PRO, it is necessary to understand some of the concepts and terminology used within the program.

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Chapter 1 Installing CODESSA PRO

1.1 System requirements:

Hardware:

Processor: Pentium class systems - minimum. All processors developed hereafter by Intel Corp. are supported on the assembly level optimization.
All AMD current processors work as old Pentium with higher clock freqency (no special optimization).

Memory: 128MB minimum, 256MB default tuning.

CD-ROM: A CD-ROM or a compatible DVD device is required to install CODESSA PRO software.

Other: A 3D graphics accelerator is highly recommended because of extensive use of OpenGL for presentation of molecules.
2-button mouse is required.

Software:

Operation system: Windows XP Professional, Windows XP Home, Windows 2000, Windows NT (with limitation on using network drives)
Workstation and Server.
On Windows ME, Windows 98 and Windows 95, the program works with many limitations and is tested not very well.
Operation system extensions: Internet Explorer 4.0 SP2 or newer version.

1.2 Installation instructions.

1. Place the CODESSA PRO CD in your CD-ROM drive.
2. If the windows Autorun feature is turned on, the installation options will be displayed automatically. If the installation options do not appear, open the Windows **Start** Menu and choose **Run**. The **RUN** dialog box opens.
3. Enter the following command in the open text box (assuming D is your CD-ROM:

   D:\setup.exe

4. Choose **OK**. The CODESSA PRO setup program initializes and the CODESSA PRO setup dialog box opens.
5. Follow the on screen instructions for product choice and installation.

The CODESSA PRO setup program will detect an existing CODESSA PRO installation and offer you the choice of uninstalling or keeping the older version of the program.

Chapter 2 Description of CODESSA PRO

2.1 Concepts and definitions

The use of CODESSA PRO requires an understanding of the following concepts:

Artifacts:

These are the individual files or items used by CODESSA PRO. There are four types of artifacts: structures, descriptors, properties, and models. Using the CODESSA PRO program will frequently require manipulation of single artifacts or lists of artifacts. CODESSA PRO names explicitly most artifacts (*e.g.* descriptors and models).

Storage:

All items that are connected with a project are stored in a single location within the file system - in the **storage**. To change a storage location, click **Option** on the main menu-bar and select **Storage**. The box that opens allows the user to control the storage location of structure files, correlations, descriptors, lists etc.

Snapshot (Cache File):

The snapshot (CODESSA PRO cache file) is a binary (compressed) representation of all items in storage. This file is located in the memory whenever work is being performed on the CVI module. The cache file reloads each time the CVI detects a change in the storage contents. The snapshot can be reloaded manually at anytime by opening the pull-down menu **Calculate** on the menu-bar, then selecting **Load storage,** or by using **F5** keyboard shortcut.

Workspace:

The **workspace** is a window within the CVI that represents the snapshot, it is located in the workspace area on the top left side of the CVI frame.

Folder:

A **folder** is used to store lists and is similar to a directory. CODESSA PRO uses four types of folders: structure, descriptor, property, and model (correlation). Each of the first three folders has a system-generated list named **All**. This list will contain “ALL” of the structures, descriptors or properties for the corresponding folder. The **Descriptors** folder also includes system-defined descriptor lists according to group and type. A particular descriptor item may be contained in several lists. The **Correlations** folder contains lists for each property item in the property folder. The list is generated automatically by the system when a property item is created. When correlations are calculated, 50 correlation items (by default) will be stored in the list that corresponds to the property.

Structure:

A **structure** is a representation of an individual chemical object with a precise chemical constitution. Examples of structures include a single molecule, a monomeric unit of a polymer, or a molecular complex with a definite composition. The minimum information that a structure must include is the types of atoms involved and their connectivity. Each structure must be linked with three files containing: 3-D structure, SCF, and Force information. Before a 3-dimensional structure can be input into CODESSA PRO, it must be converted to MDL *molfile* format and be optimized. The *molfile* structures are stored in the **3D MOL(MOPAC) Subfolder**, SCF output files are stored in the **SCF Subfolder**, and Force output files are stored in the **THERMO Subfolder**. SCF and Force structures will be created and properly stored automatically by the CMol3D module. See **Starting a New Project** for instructions to create each file type. It is vital that the name for a particular structure be exactly the same in each directory. Structure names must be in the form Sddddddd.xxx and should be added in sequential order (e.g. S0000001.xxx, S0000002.xxx…), which will be produced automatically by CODESSA PRO.

Descriptors:

Descriptors are defined as numerical characteristics associated with chemical structures. They are derived from the structures’ chemical constitution, topology, geometry, inherent wavefunction, potential energy surface or some combination of these items. The values of a particular **descriptor** can be provided by the user or calculated by the CODESSA PRO program. Each **descriptor** value must be associated with a previously defined **structure**. Descriptors calculated by the CODESSA PRO program are named automatically; renaming descriptors is not recommended.

Property:

Property is a physical or chemical characteristic, biological activity, or other characteristic of interest. Each property value must be associated with a **structure** located in the Structure folder.

Descriptor/Property Matrix:

The descriptor/property matrix consists of descriptor (all columns except the last) and property (the last column) values. The horizontal dimension of the matrix is the descriptor/property ID sequence and the vertical dimension is the structure ID sequence. The matrix has two presentations: binary and text. The binary presentation is used for internal use, while the text presentation is optimized for import into the STATISTICA and other software package at present in the CSV format.

Current Analysis Dimensions:

The dimensions used for an analysis by CODESSA PRO are the property, the list of descriptors, and the list of the structures. All the dimensions are selected by right clicking the dimension desired; this will open a context pop-up menu, from which should be chosen **make current;** the one chosen will be in boldface font to indicate that it is the currently selected dimension. The default dimensions for a new snapshot file are:

Dimension	Default value
Property	First selected
List of descriptors	**All** group
List of structures	**All** group

The selected dimensions are used in the formation of the descriptor/property matrix.

Correlation:

A **correlation** represents the results of a (multi)linear regression between a property of interest (y) and one or more selected descriptors (x_i).

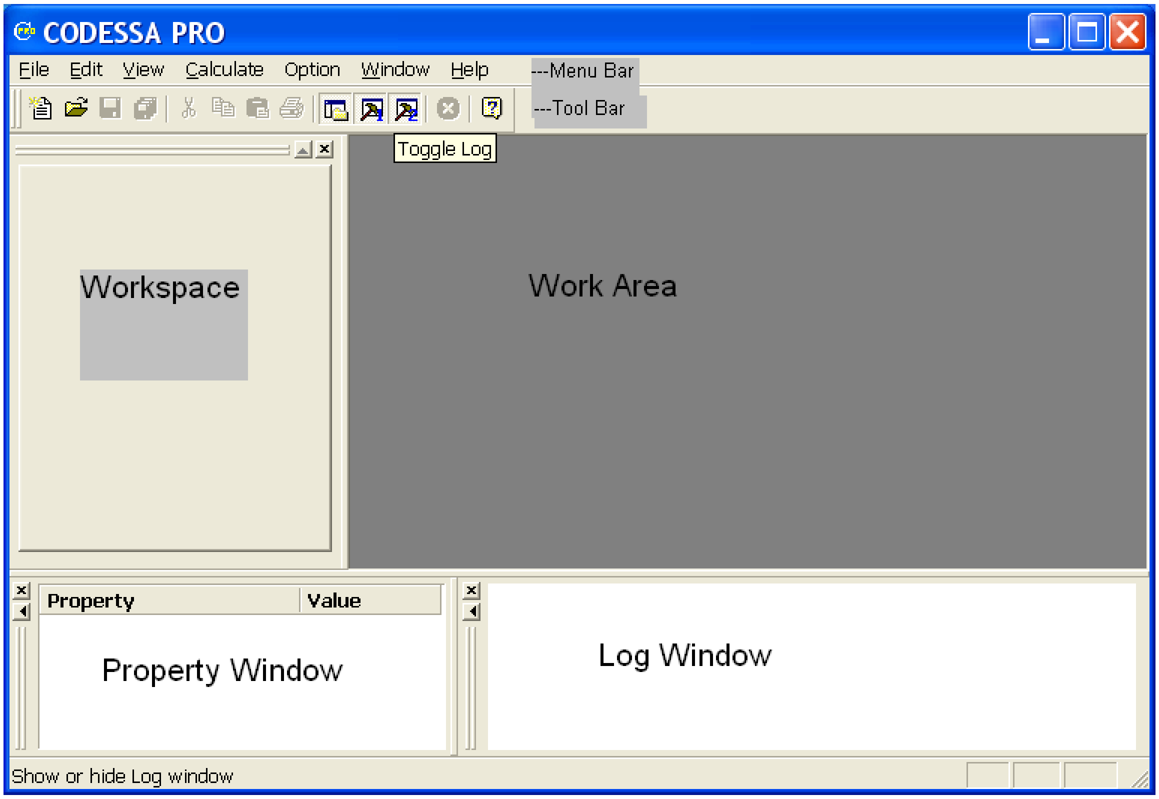
$$y = a_0 + \sum a_i x_i$$

Correlations are composed of regression coefficients (a_i), a correlation coefficient (R^2), a squared standard deviation (s^2) and a Fisher criterion F value for the set of structures used in the derivation of the correlation. By default, each **correlation** is named by its number of structures (N), correlation coefficient (R^2), crossvalidated correlation (R^2_{CV}) and Fisher criterion value (F), and squared standard deviation (s^2).

List:

A **list** is collection of the chemical structures, descriptors, physical and chemical or other property of interest, or models (correlations). Lists can be either system type or user type. System lists cannot be deleted by the user. To select the items that it is desired to include in a new list, right click to show a context pop-up menu, and then choose **create list** to make a new list. To delete a list, click the list that you want to delete, right click to show a context pop-up menu, and then choose **delete list.**

2.2 CODESSA PRO Visual Interface



Workspace: An on-screen presentation of the current cache file.

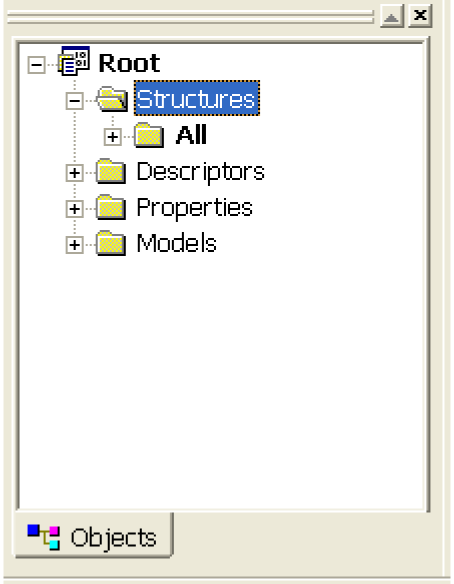
Work Area: The screen space for various view windows.

Property Window: The property window depicts information about properties of the selected object and is available for almost all objects.

Log Window: The window’s purpose is protocol all operation on the storage.

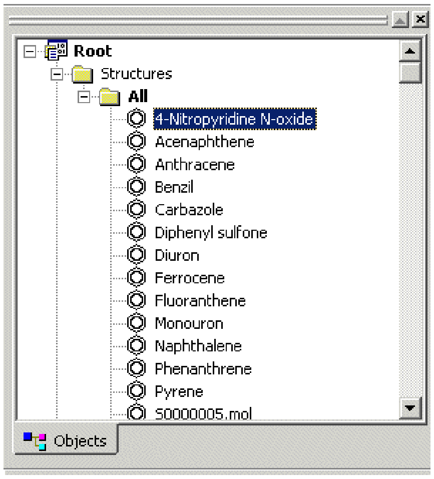
Tool Bar: Shortcuts to commonly performed tasks. The task will be displayed when the pointer is positioned over the icon.

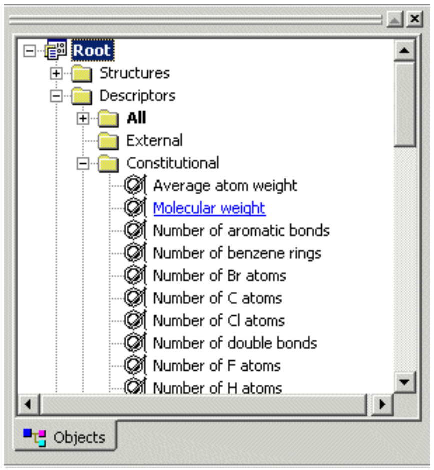
2.2.1 Workspace



The workspace area contains an on-screen presentation of the current cache file which is essentially a directory tree. Clicking on the minus will collapse a folder (branch of the tree) and clicking on a plus will expand a folder. When a folder is expanded (note the **structures** folder) it will show the lists (note **All** list) contained in the folder. The same icon is used to represent lists as folders because they are also used to contain files. If a list is empty then there will be no plus or minus beside it.

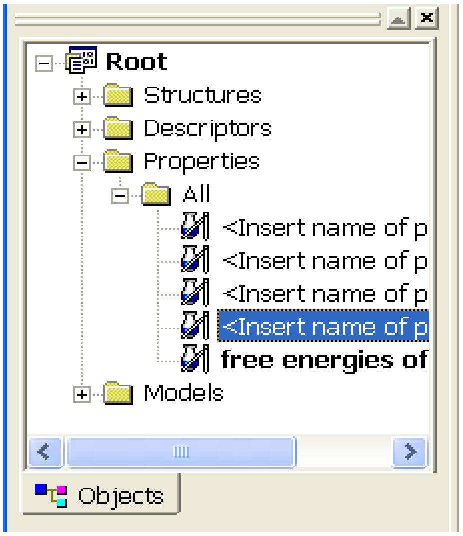
The **Structures** folder is expanded to show the list **All**. The list **All** is also expanded to show the structure artifacts. Notice the icon beside the structure artifact. Each type of artifact will have a different icon. The name that is listed will be the same as the name given on the first line of the molfile. The last structure artifact gives the filename of the molfile because the name was not entered on the first line of the molfile. Double clicking on an artifact launches a **structure view** window in the **work area**.



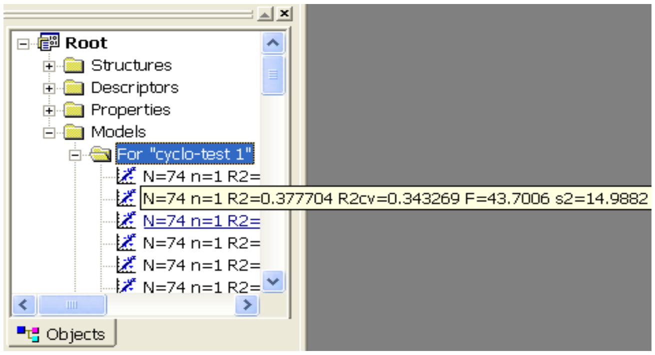


The **descriptors** folder is expanded to show the **All**, **External**, and **Constitutional** lists as well as several other descriptor artifacts. The **All** list is in boldface font because it is the currently selected analysis dimension for descriptors. Notice the descriptor icon is different from the structure icons pictured above. If an artifact is selected, its color will change from black to blue.

The **Properties** folder is expanded to show the **All** list and several property artifacts. Notice that the fifth property is in boldface font, which indicates that it is the property dimension currently selected. Notice the icon used to represent property artifacts. The name of the property artifact is the same name given on the first line of the property (P0000005.prp) file. As you can see in the picture, the first four property files are named “<insert name of property here>”. This is because all these four property files are presently empty, therefore the first line of these property files is now “<insert name of property here>”. You can alter the property files’ name by double click the current name and then changing it.

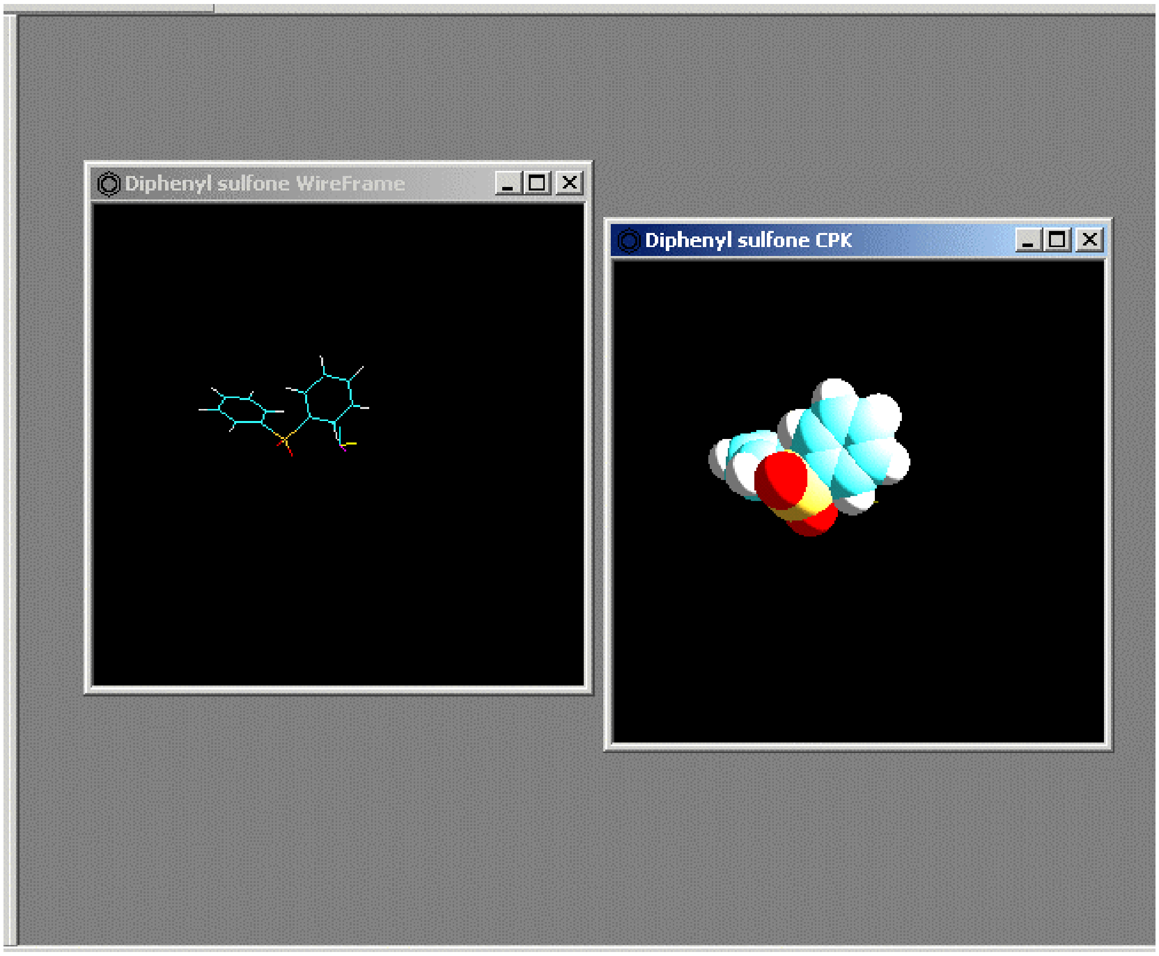


The **models** folder has been expanded to display several lists and artifacts. A list is created automatically for each property artifact. If the pointer is held over a correlation artifact, the details of the artifact are displayed. Double clicking on an artifact launches **correlation view**.



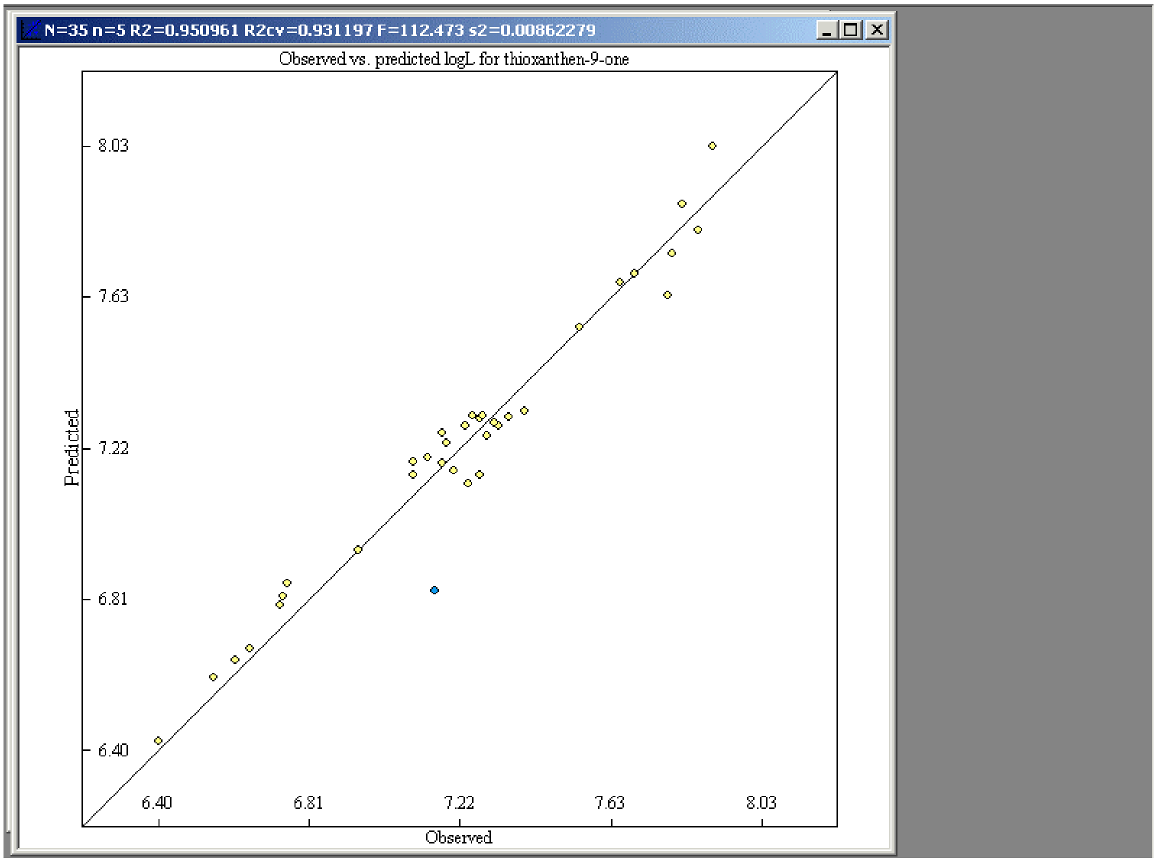
2.2.2 Work Area

2.2.2.1 Structure View Window



Double clicking on a structure artifact in the structures folder opens a **structure view window** in the work area. Structures are 3-dimensional and can be viewed as wire-frame, ball and stick, CPK surface, solvent accessible surface (SASA), Zefirov's charges on SASA (solvent accessible surface area) and MOPAC charges on SASA(solvent accessible surface). Right clicking inside the window opens the view and label context pop-up menu. Selecting **view** provides the six options mentioned above, and the label identifies the number or the type of each atom. When the pointer is positioned over the view window, it changes to a 4-sided arrow that can be dragged to rotate the structure.

2.2.2.2 Correlation View Window

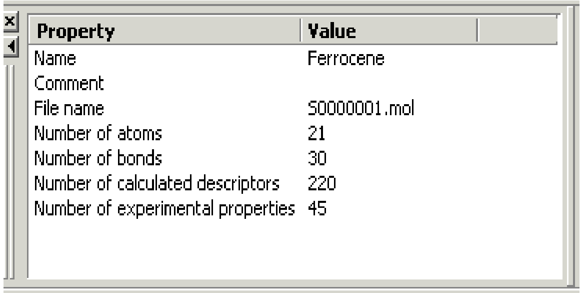

N=35 n=5 R2=0.950961 R2cv=0.931197 F=112.473 s2=0.00862279
Observed vs. predicted logL for thioxanthen-9-one
Predicted
8.03
7.63
7.22
6.81
6.40
6.40
6.81
7.22
7.63
8.03
Observed

Double clicking on a correlation artifact opens the **correlation view window**. The graph shows the observed (experimental) values versus the predicted values of the property in question. When the window is first opened, all the points for outliers will be blue rather than yellow. The color of the points will change to blue to indicate they have been selected. Clicking once on a point will display its properties and their associated values in the properties window. Double clicking on a point will open in the work area a **structure view window,** for the structure that corresponds to that point. Right clicking the window will open a context pop-up menu that will give the opportunity to **show structures**, **show descriptors**, create Sublists, mark outliers and mark non-outliers as desired.

Double clicking on a descriptor artifact will also open a **correlation view window**. The window will show the relationship between the descriptor and the property dimension selected. The value predicted according to any model chosen maybe viewed by selecting that model, clicking the **view** pull-down menu, and then choosing **predicted properties**. This will display the observed property values, predicted property value and errors.

2.2.3 Property Window

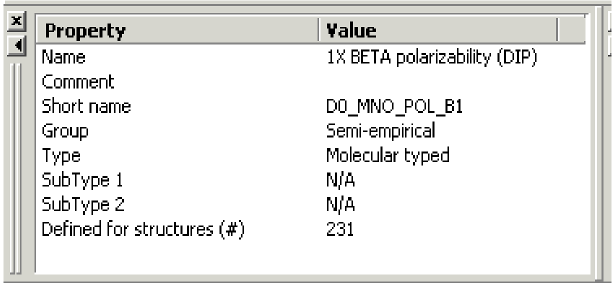
The item selected determines the contents of the property window. If a folder or list is selected in the workspace, the number of artifacts contained is displayed. If an artifact is selected, the **property window** will provide varying information, depending on the type of artifact.



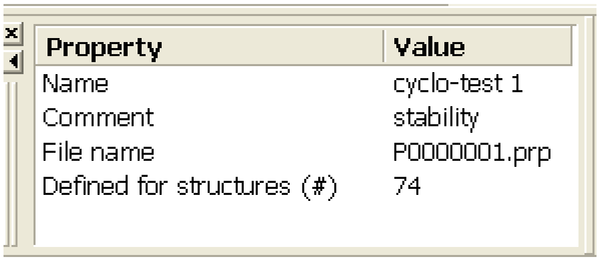
Property	Value
Name	Ferrocene
Comment	
File name	S0000001.mol
Number of atoms	21
Number of bonds	30
Number of calculated descriptors	220
Number of experimental properties	45

The picture on the left shows the information given in the **property window** when a structure artifact is selected. It will also show the experimental value and calculated value of the property of the current structure, which are not shown in the picture now.

The picture shows the information provided when a descriptor artifact is selected in the workspace.

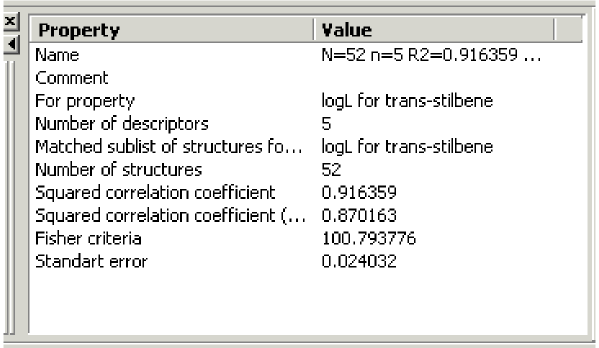


Property	Value
Name	1X BETA polarizability (DIP)
Comment	
Short name	D0_MNO_POL_B1
Group	Semi-empirical
Type	Molecular typed
SubType 1	N/A
SubType 2	N/A
Defined for structures (#)	231



Property	Value
Name	cyclo-test 1
Comment	stability
File name	P0000001.prp
Defined for structures (#)	74

When a property artifact is selected, information from the prp file is displayed. This includes name, comments and the number of structures.

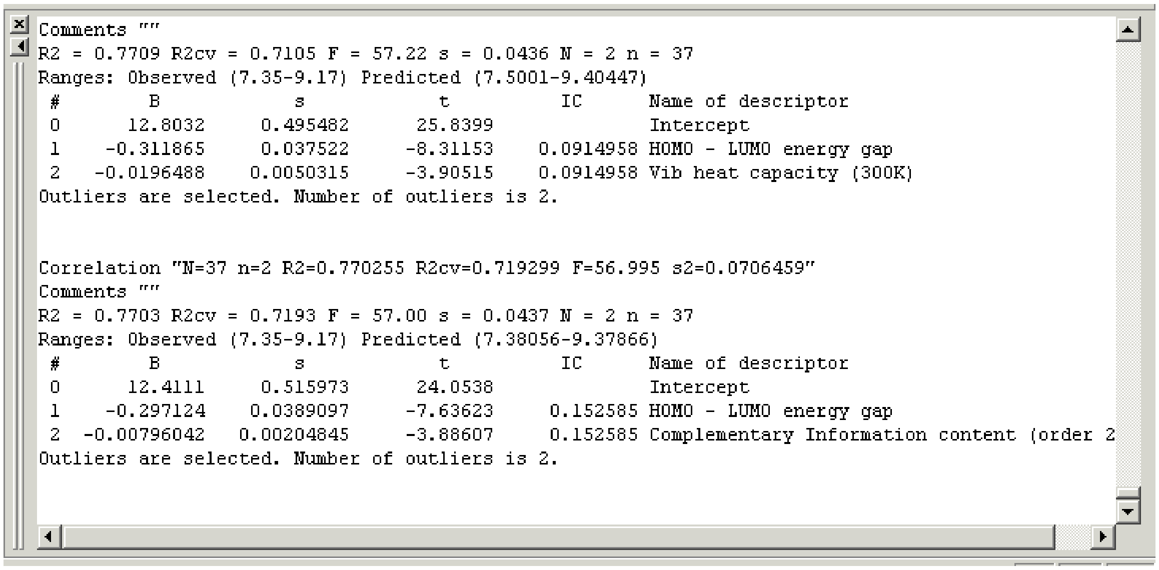


Property	Value
Name	N=52 n=5 R2=0.916359 ...
Comment	
For property	logL for trans-stilbene
Number of descriptors	5
Matched sublist of structures fo...	logL for trans-stilbene
Number of structures	52
Squared correlation coefficient	0.916359
Squared correlation coefficient (...	0.870163
Fisher criteria	100.793776
Standart error	0.024032

The **property window** for correlation artifacts lists the details of the correlation. Details displayed include the properties used in the correlation.

2.2.4 Log Window

The **log window** describes each operation that has been performed on the storage. Double clicking on a correlation in the workspace will give a full description of the correlation (as pictured below). The text is in RTF format and can be cut and pasted directly into a word processing program.



```
Comments ""
R2 = 0.7709 R2cv = 0.7105 F = 57.22 s = 0.0436 N = 2 n = 37
Ranges: Observed (7.35-9.17) Predicted (7.5001-9.40447)
 #        B            s            t          IC      Name of descriptor
 0      12.8032     0.495482      25.8399              Intercept
 1    -0.311865     0.037522     -8.31153    0.0914958 HOMO - LUMO energy gap
 2   -0.0196488    0.0050315     -3.90515    0.0914958 Vib heat capacity (300K)
Outliers are selected. Number of outliers is 2.


Correlation "N=37 n=2 R2=0.770255 R2cv=0.719299 F=56.995 s2=0.0706459"
Comments ""
R2 = 0.7703 R2cv = 0.7193 F = 57.00 s = 0.0437 N = 2 n = 37
Ranges: Observed (7.35-9.17) Predicted (7.38056-9.37866)
 #        B            s            t          IC      Name of descriptor
 0      12.4111     0.515973      24.0538              Intercept
 1    -0.297124    0.0389097     -7.63623     0.152585 HOMO - LUMO energy gap
 2  -0.00796042   0.00204845     -3.88607     0.152585 Complementary Information content (order 2
Outliers are selected. Number of outliers is 2.
```

The **edit** pull-down menu has options to **select all log, copy from log, paste to log** and **clear all log**. Transferring the information for several correlations to a word processing program can be accomplished by **clearing all log**, double clicking on each of the correlations, then clicking **select all log**, finally **copy from log**.

Chapter 3 Using CODESSA PRO to start a new project

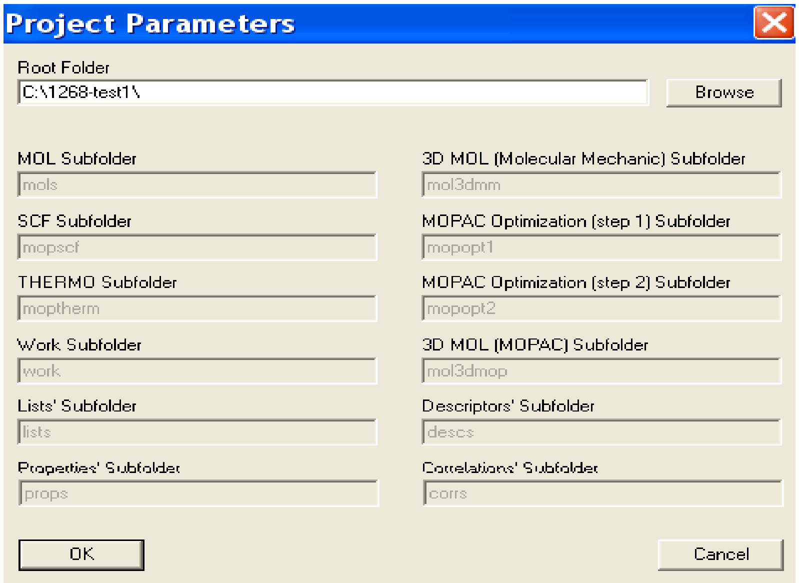
3.1 Creating a new folder for the new project

You can select the drive on which it is desired to save the data, and then make a new folder which can be named either by project number or any other way of your choosing.

3.2 Creating a storage list

You have two choices for creating a storage list, either one for many projects or just for one individual project. If you decide to use a single storage list for many projects, you must keep an index of the structure and molecule names. Although a general storage for many projects allows a research group to avoid repeating the calculations of structures and descriptors as well as to minimize the amount of storage space used, we strongly recommended the use of separate storage list for each project.

To create storage for a new project, click the **option** pull-down menu, click **storage,** and **browse** to find the folder that has just been created for your storage. Then, click **OK** to close the window. Now, in the project folder you will find a subfolder list, an example of which appears in the following picture. You can name each folder in many desired manner or use the default names which shown in the shaded area.



Project Parameters

Root Folder: C:\1268-test1\

MOL Subfolder: mols

3D MOL (Molecular Mechanic) Subfolder: mol3dmm

SCF Subfolder: mopscf

MOPAC Optimization (step 1) Subfolder: mopopt1

THERMO Subfolder: moptherm

MOPAC Optimization (step 2) Subfolder: mopopt2

Work Subfolder: work

3D MOL (MOPAC) Subfolder: mol3dmop

Lists' Subfolder: lists

Descriptors' Subfolder: descs

Properties' Subfolder: props

Correlations' Subfolder: corrs

All the storage subfolders should be empty before starting any optimization or calculation. First, you need to prepare .mol files of your structures and save them either in the **MOL subfolder** or in a location of your choosing. Keep in mind, no matter how you name your .mol files, whenever you run CODESSA PRO, the program will automatically name the files as Sddddddd.mol.

3.3 Preparing storage

Compared with old CODESSA, a major enhancement achieved by CODESSA PRO is that CODESSA PRO is highly automatic, and this obviates manual storage preparation.

Since you already have all the .mol files of all the structures, if you save your .mol files in the **MOL Subfolder**, pressing **F5** keyboard shortcut automatically prepares all the data which are necessary for doing correlation. If the location of your .mol files is different, then select the **edit** pull-down menu, choose **add structure**, browse for the folder where your .mol files are located and click **ok**.

The process through which CODESSA PRO prepares all the data, except property files, is divided into 11 stages. Each of these 11 stages is performed automatically in sequence by CODESSA PRO.

Stage 1

This is the first model building stage. The program applies simple molecular mechanics preoptimization and transfers the 2-dimensional structures from the **MOL** subfolder to the 3-dimensional structures that will be stored in the **3D MOL (Molecular Mechanic)** subfolder. Missing hydrogen atoms are added according to the formal valence rules. The model building is done deterministically for the first iteration and stochastically for subsequent iterations.

Stage 2

This stage is concerned with the conversion of the file from MDL MOL format in the **3D MOL (Molecular Mechanic)** subfolder into the MOPAC input file format for preliminary geometry optimization in the **MOPAC Optimization (step1)** subfolder.

Stage 3

This stage performs the preliminary geometry optimization using CMOPAC (MOPAC Version 7 clone). If the gradient is less than 5.0, the program automatically proceeds to **Stage 4**. If the gradient is more than 5.0, then the program automatically go back to **Stage 1** and starts model building again, stochastically. This process is continued up to 10 times until the optimization stage is passes on the criteria of the gradient value being less than 5.0. If success is not achieved after 10 iterations, then program stops.

Stage 4

During this stage, the program converts the MOPAC output files in the **MOPAC Optimization (step1)** subfolder into a MOPAC input file for precise geometry optimization, and stores them in the **MOPAC Optimization (step2)** subfolder.

Stage 5

CODESSA PRO is performing precise geometry optimization at this stage. If the gradient value can be reduced to less than 0.5, then the program proceeds automatically to **Stage 6**. If the gradient is more than 0.5, then CODESSA PRO goes back to **Stage 1** and does model building again, stochastically. This process is continued up to 10 iterations until the gradient value test for the precise optimization is satisfied. If 10 iterations are unsuccessful, the calculations are stopped.

Stage 6

At this stage, the CODESSA PRO program converts the MOPAC output files in the **MOPAC Optimization (step2) Subfolder** into MOPAC input files for calculation of molecular properties. It is possible to do this without calculation of the Hessian matrix. The resulting MOPAC input file is stored in **SCF Subfolder**.

Stage 7

Next, at stage 7, the CODESSA PRO program produces a set of molecular properties calculated using CMOPAC. MOPAC input files. The resulting output files are stored in the **SCF Subfolder.**

Stage 8

Next, CODESSA PRO program takes the molecular geometries in the **MOPAC Optimization (step2) Subfolder**, prepares MOPAC input files for force calculations, and stores them in the **THERMO Subfolder**. At this stage keyword ROT=1 is added, which is valid for C1, CI, and CS groups of symmetry (This applies to almost all organic molecules). However, If molecular symmetry is different from point groups C1, CI, and CS mentioned above, the keywords need to be edited manually. To achieve manual editing, open the .mni files in **MOPAC Optimization (step1) Subfolder** or **MOPAC Optimization (step2) Subfolder** with **Notepad** or W**ordpa**d, and then add the desired keywords.

Stage 9

At this stage, CODESSA PRO program calculates the molecular properties using the Hessian matrix ("force" calculation). The state of the molecule is determined using the signs of eigenvalues of the Hessian matrix. If the molecule are in a transition state, than the program goes back to **Stage 1** and restarts by using stochastic addition again. If the molecule is in its ground state, then go to **Stage 10**. If 10 iterations are unsuccessful, stop calculation.

Stage 10

This stage will be reached only in situations when all mentioned the geometry tests above are satisfied. At this stage, the MDL MOL file in the **3D MOL (MOPAC) Subfolder** is formed, based on formal connectivity information from the MDL MOL file in the **MOL Subfolder,** and atomic coordinates from the MOPAC output file in the **MOPAC Optimization (step2) Subfolder**.

Stage 11

CODESSA PRO takes all MDL MOL files in the **3D MOL (MOPAC) Subfolder**, the MOPAC output file in the **SCF Subfolder** and the MOPAC output file in the **THERMO Subfolder** to do descriptor value calculations. The resulting text file with descriptor values is stored in the **Descriptor's Subfolder**. All intermediate files are deleted from storage at this stage. Only MDL MOL files in the **MOL Subfolder** and the **3D MOL (MOPAC) Subfolder,** and MOPAC input and output files in the **SCF Subfolder** and **THERMO Subfolder** remains.

If the calculation cycle is not finished at **Stage 1**, changes can be made to the files at the last successful stage manually (usually it is editing of MOPAC keywords) and the calculations restatred. If four files (MDL MOL files in the **MOL Subfolder** and the **3D MOL (MOPAC) Subfolder,** and the MOPAC output files in the **SCF Subfolder** and the **THERMO Subfolder)** are present and up-to-date, no further calculation will be done. The up-to-date state is defined using the modification time of the files. In case it is not, the calculations will be processed starting from the most recently corrected file. To invoke the recalculation, select from the menu **Calculate/Load Storage (F5)** or **Calculate/Descriptors (F6)**. In the last case, only problematic structures which show in **MOPAC Optimization (step1) Subfolder** and **MOPAC Optimization (step2) Subfolder** will be recalculated. If the problems arise as a result of a structure's improper format, you must redraw the structure in the **MOL Subfolder**.

Note:

Before a correlation is run, you should check if everything in the storage is ready. All subfolders in the storage should be empty except the following:

1. **MOL Subfolder**- this subfolder should contain all .mol files of all structures.

2. **SCF Subfolder**- this subfolder should contain only .mni and .mno files of all structures.
3. **THERMO Subfolder**- this subfolder should contain only .mni and .mno files of all structures.
4. **3D MOL (MOPAC) Subfolder**- this subfolder should contain only .mol files of all structures which are different .mol files from the mol files present in the **MOL Subfolder**.

Preparing property files

If the above is accomplished satisfactorily, the final requirement prior to correlation is to prepare the property files. On the CODESSA PRO window, click the **edit** pull-down menu and choose **add property**. Then you input the name, comment, and property value according to the format which is indicated in the notepad, and finally, use the **F5** keyboard shortcut for CODESSA PRO to load the data.

3.4 Calculating the correlation.

Ensure that structures, descriptors, and properties of interest are selected (they should all appear in boldface font). If not, right click the name of structures, descriptors or property to show a context pop-up menu, then select **make current** to highlight them .Click on the **calculate** pull-down menu and choose **HMPRO,** or just press the **F9** keyboard shortcut instead. The correlation will be finished automatically by CODESSA PRO. If you just want to calculate descriptors, then click on the **calculate** pull-down menu and choose **descriptors,** or press the **F7** keyboard shortcut instead. You can also choose **form matrix** which in addition to descriptor calculation will also form a matrix. You can limit the maximum number of descriptors for your model by clicking on the **option** pull-down menu, choosing **HMPRO**, clicking **expanding**, then inputting the maximum number of descriptors you permit in your model.

3.5 Viewing correlations

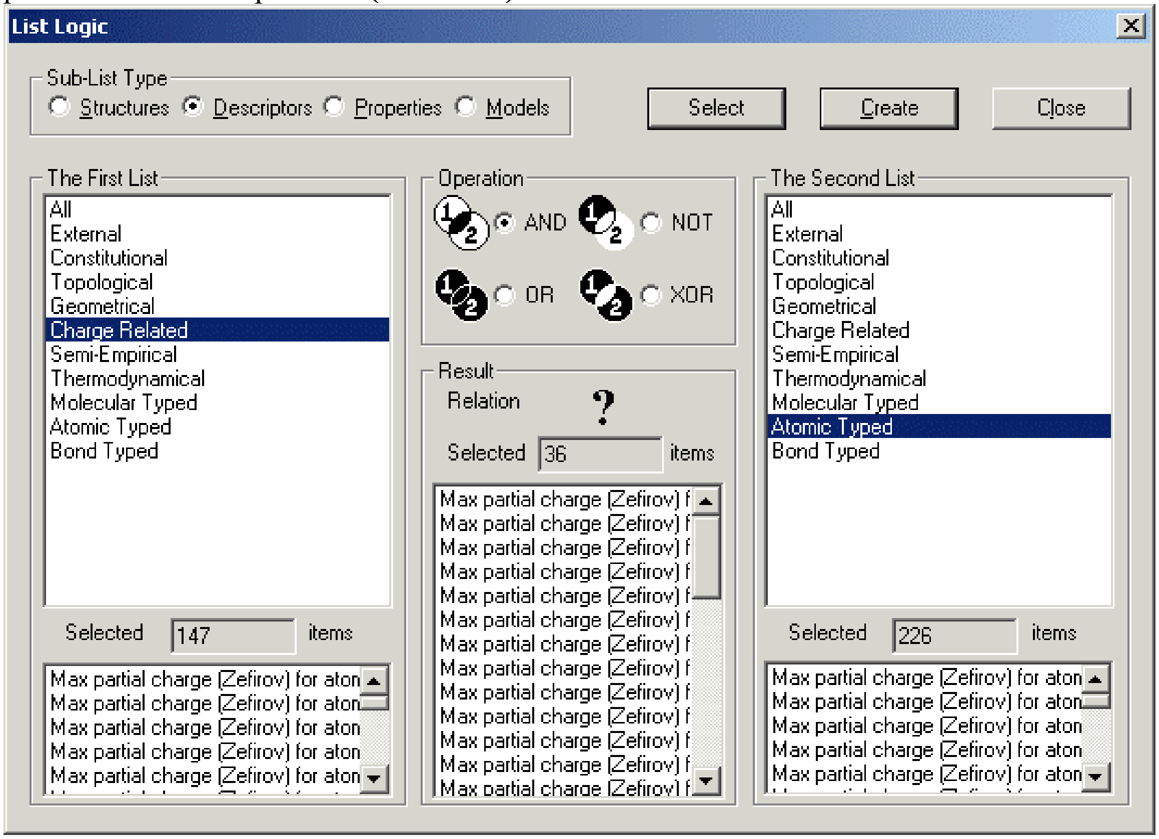
When the correlations are finished, you just double click **mode**l and all the models respond to each property file will show up. Then you double click the model that you want to take a look to open the **correlation view window** (see page 17)

3.6 Printing your results.

Use **prin**t from the **file** menu bar to print the correlation plot from the **work area**. To print information from the **log area**, follow the instructions given on page 19 and then print from the corresponding word processing program.

3.7 Manipulating lists

CODESSA PRO automatically produce one or more lists in each folder, but when analyzing a property or correlation, it is sometimes helpful to create a user-defined list, e.g. a list of structures containing phenyl rings. The simplest method for creating a list in CODESSA PRO is to select several artifacts from one or more existing lists (i.e. **all**), right click to open the context pop-up menu and left click on **create list**. A list can also be formed from a group of artifacts that are linked to a *common* artifact. If a descriptor is chosen to be the *common* artifact, then all the structures that are defined for that descriptor could be selected for a list. To create the list from a *common* artifact, select the *common* artifact, open the context pop-up menu, click on **Select Linked**, and then select the type of artifacts that you want to add to the list. To create a list from multiple *common* artifacts, select the list that is created corresponding to each *common* artifact, then perform the **AND** operation **(**see below**)**.



Sub-List Type
○ Structures ● Descriptors ○ Properties ○ Models

The First List
All
External
Constitutional
Topological
Geometrical
Charge Related
Semi-Empirical
Thermodynamical
Molecular Typed
Atomic Typed
Bond Typed

Selected 147 items

Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton

Operation
● AND ○ NOT
○ OR ○ XOR

Result
Relation ?

Selected 36 items

Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f
Max partial charge (Zefirov) f

The Second List
All
External
Constitutional
Topological
Geometrical
Charge Related
Semi-Empirical
Thermodynamical
Molecular Typed
Atomic Typed
Bond Typed

Selected 226 items

Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton
Max partial charge (Zefirov) for aton

The **List Logic** module in CODESSA PRO compares the artifacts contained in two lists and can be opened by clicking any artifact, right clicking to show the context pop-up menu, and choosing **lists logic,** or just using the **F4** keyboard shortcut instead**.** Choose the type of artifact that will be contained by the list by clicking on the appropriate button in the **Sub-List Type** box (**descriptors** is selected in the example above). Choose the desired lists for comparison and the appropriate **Operation**. The artifacts from the two lists that meet the criteria of the operation will be displayed in the **Results** box. The results can then be copied to a new list (**Create**) or be selected (**Select**) for further comparison. When comparing three or more lists, first compare two of the lists, click on **Select**, restart **List Logic**, select **Current Selection** in **The First List** box, then select the remaining list in **The Second List** box.